Python & In-memory CGNS trees

Using CGNS trees for Code-coupling

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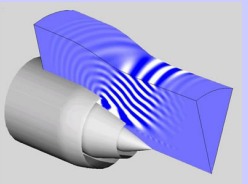
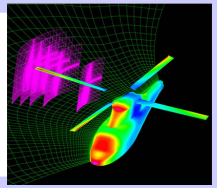
Code life cycle



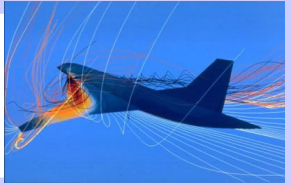
- Idea/Code/Test/Change
  - Prototype
  - Test
  - Pre/Post processing
  - Code-coupling
  - Parallel
  - All you can do with another programming language
    - Interpreted
    - Actually dedicated to code gluing
    - Script languages are easily extensible
- Baseline for an Open System

Python



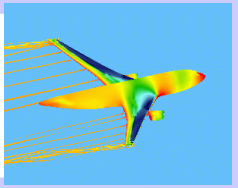
- Object-oriented interpreted language
  - Very easy to learn
  - Clear syntax
  - Powerful numerical extensions
    - Python/C/C++/Fortran arrays
- Good candidate for code gluing
  - Pre & post processing on CGNS data
  - A scripting language

pyCGNS



- Python wrapper on CGNS MLL and ADF
  - Straightforward mapping
  - Use 100% python types
    - Lists, strings, integers, floats
    - Numerical array
      - Contiguous C/Fortran array
      - Points to actual memory zone
- Easy scripting
  - Perform CGNS calls on-the-fly

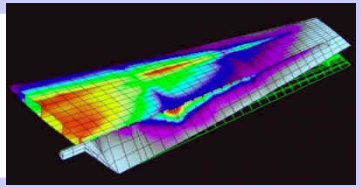
Python/CGNS tree



- Tree representation
  - List of nodes
  - Each node has...
    - A Name
    - A Type
    - A Value
    - A list of sons
  - Generic CGNS low level node requirements (ADF/HDF5)

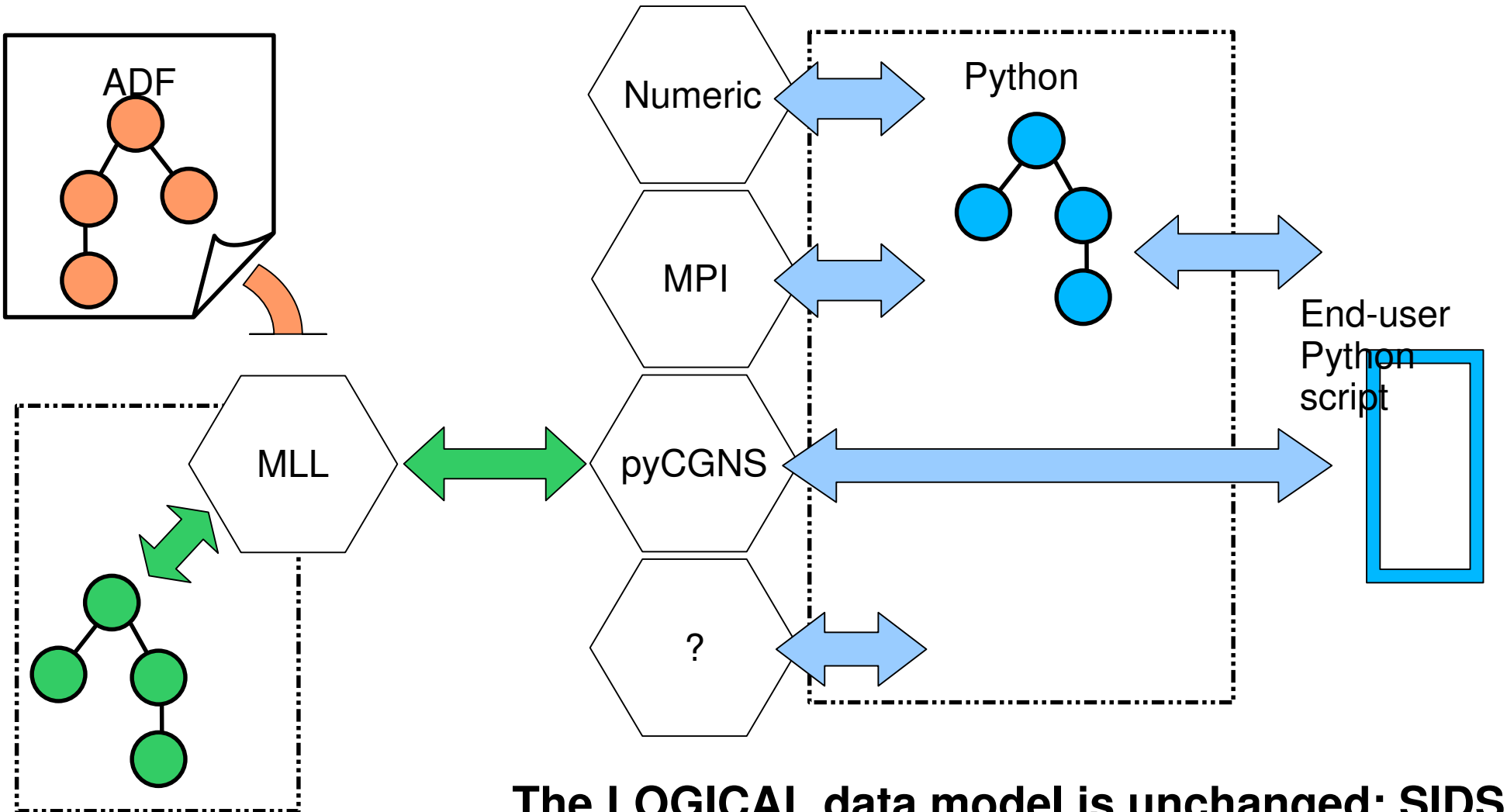
```
['Transform',(1, 2, 3),[],'int[IndexDimension]'],
['PointRange',((1, 1, 1), (1, 9, 9)),[],'IndexRange_t'],
['PointRangeDonor',((21, 1, 1), (21, 9, 9)),[],'IndexRange_t']
```

File and memory



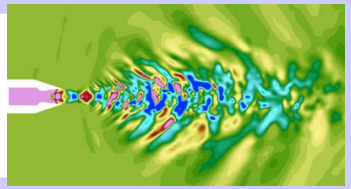
- ADF/HDF5 file
  - open/read/write/close
  - MLL keeps private tree structure in memory
  - ADF is per-node but still private data structure
  - PyCGNS only maps to this behaviour
- Python tree
  - The Python/CGNS tree is just another implementation
  - Structure in memory but not a proprietary one
  - Same interface/Different implementation

File & memory workflow



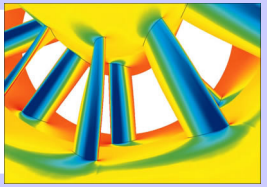
The LOGICAL data model is unchanged: SIDS

pyCGNS example



```
import CGNS
import numarray as N

x=y=z=N.zeros((3,5,7),'d')

a=CGNS.pyCGNS("newfile.cgns",CGNS.MODE_WRITE)

print a.error

idb=a.basewrite("Base",3,3)
idz=a.zonewrite(idb,"Zone 01",[3,5,7],CGNS.Structured)

a.coordwrite(idb,idz,CGNS.RealDouble,CGNS.CoordinateX,x)
a.coordwrite(idb,idz,CGNS.RealDouble,CGNS.CoordinateY,y)
a.coordwrite(idb,idz,CGNS.RealDouble,CGNS.CoordinateZ,z)

a.close()
```

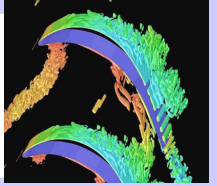
Scripting example: Prototypes



- Can I do this and that with CGNS ?
  - Just try it !
  - Versatile testing support

```
import CGNS

f=CGNS.pyCGNS("hydro-result.cgns",CGNS.MODE_WRITE)

f.basewrite("MASS2",3,3)
f.zonewrite(1,"Block01",(2,3,4,1,2,3,0,0,0),CGNS.Structured)
f.solwrite(1,1,"07-01-1944 06:00:00",CGNS.CellCenter)
f.fieldwrite(1,1,1,CGNS.RealDouble,"sediment",w)
f.goto(1,[(CGNS.Zone_t,1),(CGNS.FlowSolution_t,1),(CGNS.DataArray_t,1)])
f.descriptorwrite("Description","Text here")
f.descriptorwrite("Units","Text here")

f.close()
```

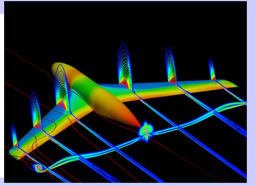
Scripting example: post-processing



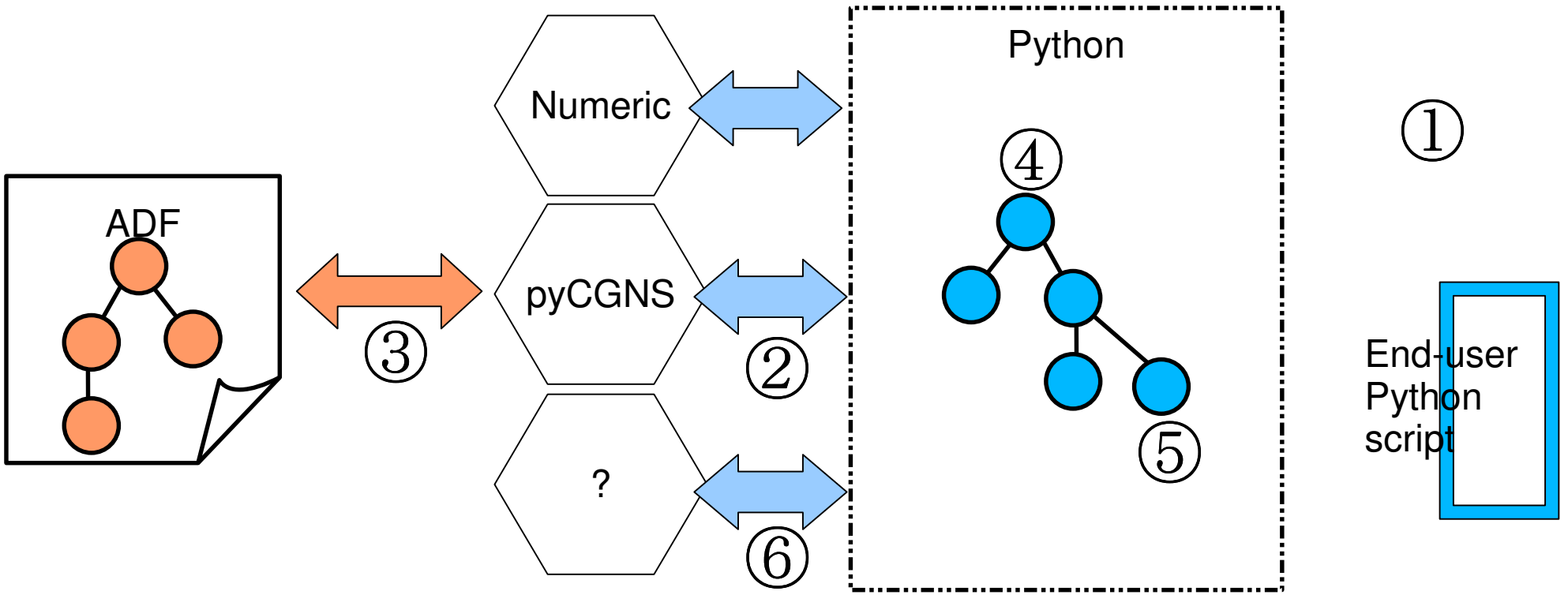
- Add links to actual grids
  - The computation sessions results are sharing the same grid
  - No duplicates
  - Post-processing adds links to the actual grid
  - True MLL/ADF calls performed on file

```
from CGNS import *

a=pyCGNS("result-001.cgns",MODE_MODIFY)

a.goto(1,[(Zone_t,1)])
a.linkwrite("GridCoordinates","grid.cgns","/Base/Zone/GridCoordinates"
)

a.close()
```

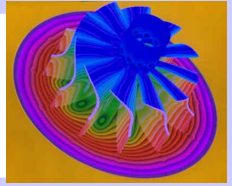
Scripting example: pre-processing



- Structured grid seen as unstructured
  - Generates connectivity
  - Read the file/Change in-memory tree/Send to code



Code-coupling



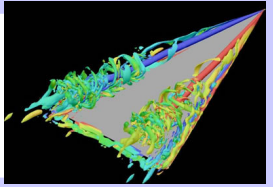
- Blind connection to peer code
  - Open System: Public interface
    - Common baseline
    - Restriction input/output
  - Use Bct for data exchange
    - Input/Output: BCDataset
    - « Contact surface »
    - Strong requirements for an arbitrary exchange mean
- Efficiency
    - Memory +no data duplication
    - Easy stub & proto

Code-coupling CGNS tree

Scripting example: code-coupling

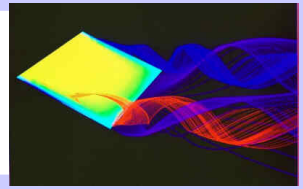
```
import MpCCI

pathB="/FlatPlate/Fluid/ZoneBC/Wall:Heat/DataSet#01/NeumannData"
pathI=pathB+"/Temperature"
pathO=pathB+"/NormalHeatFlux"
it=E.iteration()

fqx=mcci.Parameter_info("Simulation_Fluid_2_Therm_Ratio",MpCCI.CCI_INT)

xp=xw.get(E.RUNTIME_TREE)
xf=X.retrieve(pathO,xp)
if ( xf and ((it % fqx ) == 0 )):
    sd1=mcci.Parameter_info("Fluid_Private_Synchro_ID",MpCCI.CCI_INT)
    ZID=mcci.Parameter_info("Global_Mesh_ID",MpCCI.CCI_INT)
    BID=1
    nnodes=len(xf[1].flat)
    if ( (it % fqx ) == 0 ):
      mcci.Put_nodes(ZID,BID,171,1,nnodes,0,None,MpCCI.CCI_DOUBLE,xf)
      mcci.Reach_sync_point(sd1)

(rC,nC)=mcci.Get_nodes(ZoneID,BoundaryID,154,1,nnodes,0,None,MpCCI.CCI_DOUBLE)
...
E.update((E.RUNTIME_TREE,rt)
```

Scripting example: parallel



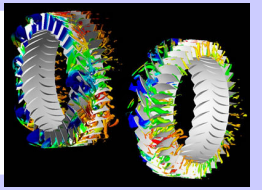
```
import elsApy    as E
from Scientific  import MPI

communicator=MPI.world.duplicate()
id = communicator.rank
if   ( id == 0 ): remoteId=1
elif ( id == 1 ): remoteId=0

datatree=E.get(E.RUNTIME_TREE)
temp=pickle.dumps(datatree)
communicator.nonblocking_send(temp, remoteId, id)
return,rank,tag=communicator.receiveString(None,None)
result=pickle.loads(return)

for l in result:
  if (l[0] == "RunTimeTree"):
    for ll in l[2]:
      if (ll[0] == "Rotor#Output"):  ll[0]="Stator#Input"
      if (ll[0] == "Stator#Output"): ll[0]="Rotor#Input"

E.update(E.RUNTIME_TREE,result)
```

In-memory issues



- Dedicated to a platform
  - One per platform: requires an API
  - Translation mandatory between platforms
    - XDR-like
- Best should be
  - Use an existing system
    - Python/Numeric (+Marshalling)
    - HDF5 (?)

Python/CGNS Tree interface



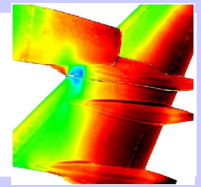
List of Python objects

- MLL-like interface
  - `NewBase`
  - `NewZone`
  - `NewGridCoordinates`
  - `NewCoordinates`
  - `NewDataArray`
- Numeric Python arrays
- Input/Output from MLL
- Use paths instead of ids
  - `GetByExactPath`
  - `GetByRegexpPath`
  - `GetAllTreePath`

```
T=CGNSTree()
base=newBase(T,"Base",3,3)
print T
getChildrenNameByPath(T,"/Base/Zone-002/GridCoordinates")
```

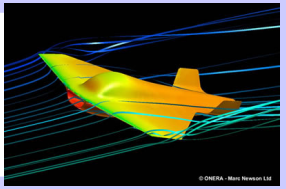
```
[['CGNSLibraryVersion', 2.4, [], 'CGNSLibraryVersion_t'],
 ['Base', array([3, 3]), [], 'CGNSBase_t']
]
```

Script example: Python/CGNS tree



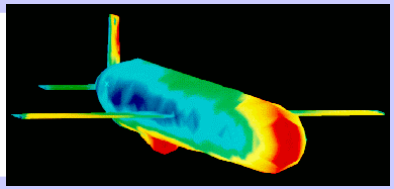
```
T=C.newCGNS()

base=C.newBase(T,"Base",3,3)
size=(20,10,5)

z1=C.newZone(base,"Zone-001",size)
C.newCoordinates(z1,"CoordinatesX",x)
C.newCoordinates(z1,"CoordinatesY",y)

f=open("T01.py","w+")
f.write(str(T))
f.close()

clist=C.getChildrenNameByPath(T,"/Base/Zone-002/GridCoordinates")
for c in clist:
  n=C.getByExactPath(T,"/Base/Zone-002/GridCoordinates/"+c)
  print C.nodeName(n)
  v=C.nodeValue(n)

print C.getChildrenType(T,"CGNSBase_t")
print C.getAllTreePath(T)
print C.getAllTreeType(T,"Zone_t")
print C.getAllTreeType(T,"DataArray_t")
```

Workflow pre/post processing



- Use tools operating on data trees
  - A data model is described by a grammar: SIDS
  - Translate the grammar for existing tools
    - Relax-NG, BNF, ...
- In-Memory data structre can be used for...
  - Perform tree verification
  - Operate tree as ADT
    - Generate code:
      - MLL/ADF/HDF5/XML/SQL/XDR/...

More than float arrays...



- CGNS is more than a storage mean...
  - CGNS as a data model
    - Store data the « CGNS way »
      - e.g. Map to 100% python objects
    - Tree with public definition
  - CGNS as component interface
    - Code-coupling data model
    - Transfer whole tree instead of arrays
      - e.g. Memory buffer based system